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Title: Large-scale molecular dynamics simulations of charged particle stopping in strongly coupled plasmas: definitive tests of plasma kinetic theories

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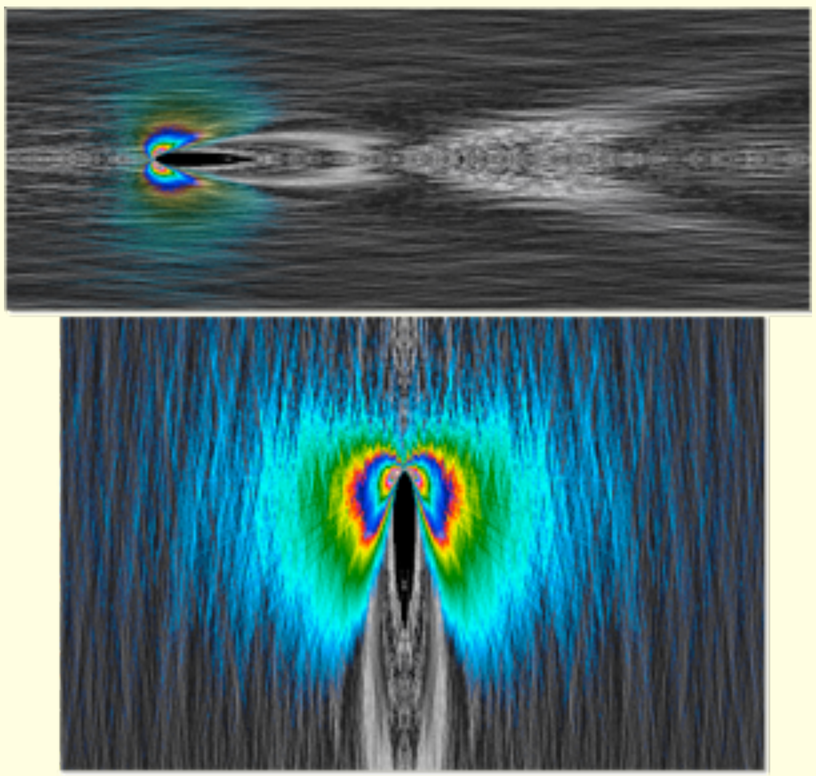
Surh, Michael P.

Intended for: Web

Large-scale molecular dynamics simulations of charged particle stopping in strongly coupled plasmas: definitive tests of plasma kinetic theories



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Thanks to the Cimarron Team

V. Batista, J. Bauer, L. Benedict, M. Calef, J. Castor, S. Chen, M. Desjarlais, I. Ellis,

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Large-scale molecular dynamics simulations of dense plasmas: The Cimarron Project

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1. Plasma kinetic theory: what would we like to know?

2. Why stopping power?

3. Physics model for molecular dynamics studies.

4. Theoretical models we chose for comparison.

5. Results.

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Some examples.

Barodiffusion:

PRL **105,** 115005 (2010) PHYSICAL REVIEW LETTERS week ending 10 SEPTEMBER 2010

Plasma Barodiffusion in Inertial-Confinement-Fusion Implosions: Application to Observed Yield Anomalies in Thermonuclear Fuel Mixtures

Peter Amendt, O. L. Landen, and H. F. Robey
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C. K. Li and R. D. Petrasso
Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
(Received 16 November 2009; revised manuscript received 23 April 2010; published 10 September 2010)

Knudsen layers:

PRL **109,** 095001 (2012) PHYSICAL REVIEW LETTERS week ending 31 AUGUST 2012

Knudsen Layer Reduction of Fusion Reactivity

Kim Molvig, Nelson M. Hoffman, B. J. Albright, Eric M. Nelson, and Robert B. Webster
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(Received 5 April 2012; published 30 August 2012)

What is the question that we wish to answer?

In kinetic theory there are two obvious limits.

Boltzmann: In a binary approximation we can employ a known, numerically-generated, or experimentally-measured cross section.

$$\mathcal{C}_B[f] = \int d\Omega d^3 p_2 \left|\mathbf{p}_1 - \mathbf{p}_2\right| \sigma(\left|\mathbf{p}_1 - \mathbf{p}_2\right|, \Omega) \left(f(\mathbf{p}_1', t) f(\mathbf{p}_2', t) - f(\mathbf{p}_1, t) f(\mathbf{p}_2, t)\right)$$

cross section = strong scattering

uncorrelated = weak coupling

Lenard-Balescu: When interactions are weak, dynamical many-body effects can be included.

$$\mathcal{C}_{LB}[f] = \frac{\pi \omega_p^4}{8\pi^3 n} \int d^3k \frac{\mathbf{k}}{k^2} \cdot \nabla_{\mathbf{v}} \int d^3v' \, \frac{\mathbf{k}}{k^2} \cdot \left(\nabla_{\mathbf{v}} - \nabla_{\mathbf{v}'}\right) f(\mathbf{v}) f(\mathbf{v}') \frac{\delta(\mathbf{k} \cdot \mathbf{v} - \mathbf{k} \cdot \mathbf{v}')}{\left|\epsilon(\mathbf{k}, \mathbf{k} \cdot \mathbf{v})\right|^2}$$

$O(e^4)$ = weak scattering

response function = dynamical correlations

- The equations complement each other: dilute and hard-collisions versus many-body and weak collisions.
- What can we do when neither of these limits applies to our problem? What regimes of plasma physics can be considered “safe”?

When must we use Convergent Kinetic Theory?

Today, we know how to remove the divergences:

1. Guess (adjust cutoffs in a Coulomb logarithm)

2. T-matrix

3. Gould-DeWitt type models

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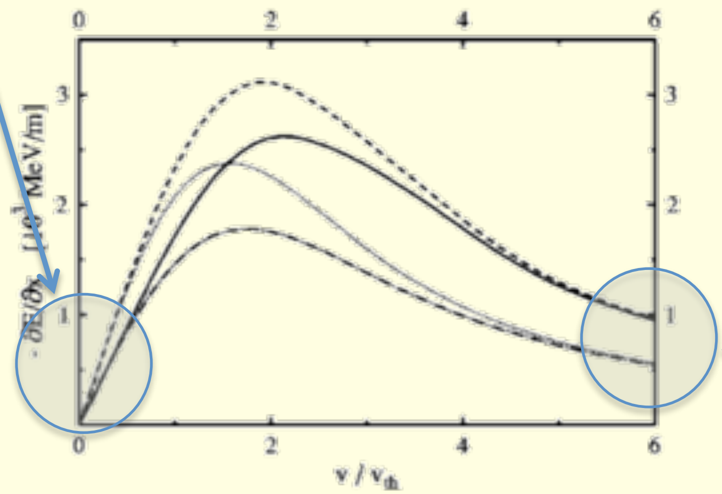
How does *velocity* impact our understanding of stopping power?

No dynamical screening: easy.



An interesting trend emerges among "reasonable" models.

Beam-plasma coupling is weak: easy.

FIG. 1. Stopping power for a proton beam in an electron gas versus beam velocity (in units of the thermal velocity $v_{th} = \sqrt{k_B T/m_e}$). The electron density and temperature are $n = 10^{21}$ cm^{-3} and $T = 5 \times 10^4$ K, respectively. The applied approximations are the RPA (dashed line), the static Born approximation (dotted line), the static T-matrix approximation (dash-dotted line), and the combined scheme (full line).

Contenders:

1. RPA (Lenard-Balescu)
2. Static Born (static screening in RPA)
3. T-matrix (static numerical cross section)
4. Combined scheme (Gould-DeWitt)

PHYSICAL REVIEW E VOLUME 60, NUMBER 1 JULY 1999

Beam-plasma coupling effects on the stopping power of dense plasmas

D. O. Gericke and M. Schlanges
Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, Domstrasse 10a, 17487 Greifswald, Germany

(Received 18 December 1998)

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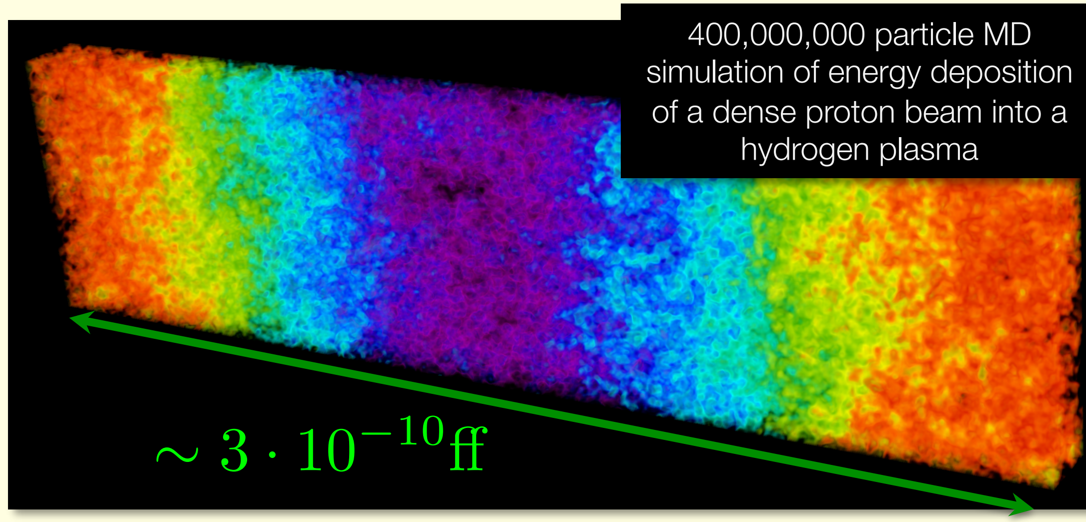
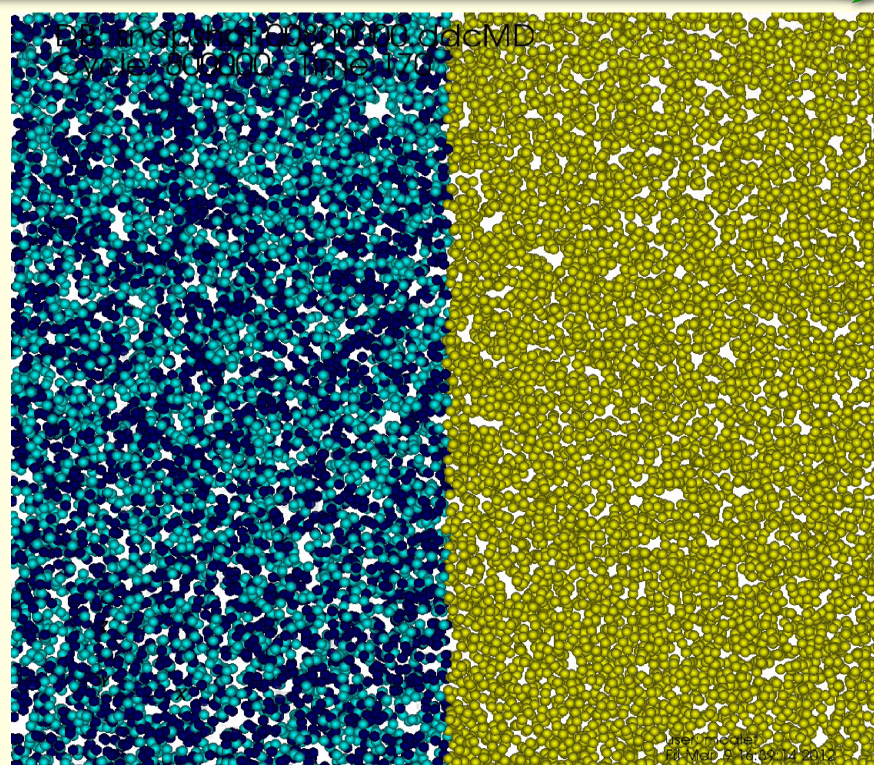
Can we formulate an interesting exact problem?



By exact, I mean:

- Numerically converged; error bars known and controlled.
- Simulation and theory are solving the same problem.



Molecular dynamics is the method of choice for collisional processes.

- Short-range forces that determine complex trajectories are treated with high precision.
- Long-range forces are also treated (Ewald, PPPM, FMM, etc.).
- Typically, second-order symplectic integrators are used (e.g., velocity-Verlet).

Alas, MD cannot do everything….

- MD is good at static quantum mechanical properties, but less is known about dynamical (i.e., kinetic) properties.
- Even where MD is good at quantum mechanics, it is always done approximately. For our purposes here*, just don't do it*!
- This weakness of MD is also its strength: classical kinetic theory is a bit harder than quantum kinetic theory. Quantum mechanics tends to smooth things out and make things easier; for example, infinities are removed in quantum mechanical models.

Statement of Problem:

- Stopping power, varying projectile velocity over a wide range.
- Perform high-accuracy, purely classical molecular dynamics.
    - N.B.: This requires the projectile charge to be the same as in the target.
- Formulate various classical collision models for comparison.

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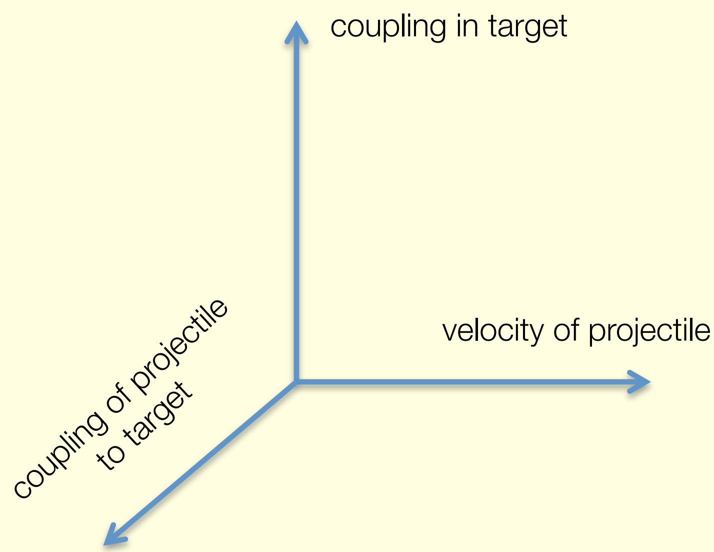
Span a Sizeable Parameter Space



$$\Gamma_{target} = \frac{e^2}{aT}$$

$$\Gamma_{proj-targ} = \frac{Z_{proj}e^2}{aT}$$

$$\tilde{\Gamma}_{proj-targ}(v) = \frac{Z_{proj}e^2}{aT\sqrt{1+(v/v_{th})^2}}$$

$$0.1 < v/v_{th} < 10$$

$$\Gamma_{target} = 0.1, 1.0, 10.0$$

$$\Gamma_{proj-targ} = 0.1, 1.0, 10.0$$

9 cases

Details of the MD Simulations

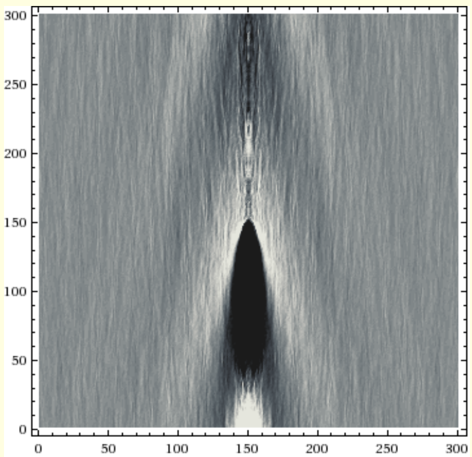
- Prior work noted that long-wavelength contributions were important, and limited the accuracy of MD, using 100-1000 particles. We used a minimum of 64,000, often 128,000, and did test runs up to 2M.
- All particles have the same sign as the target: Z=-1, -2, -10.
- Even with such large runs, wakes from periodic neighbors affected the projectile. Target was equilibrated, and projectile sent in at an angle incommensurate with the simulation cell so that it would not ride in its own wake.
- After the projectile equilibrated with the target, we collect data. We focused on energy loss per unit length, although everything is available (e.g., straggling, blooming, etc.)
- We do not wait to the particle to come to a stop: we perform many simulations for different initial velocities. But, we do perform a number of runs at each initial velocity to get error bars.
- Heating of the projectile was minimized by having many particles in the target and through the use of a weak Langevin thermostat.

Images of the simulation cell

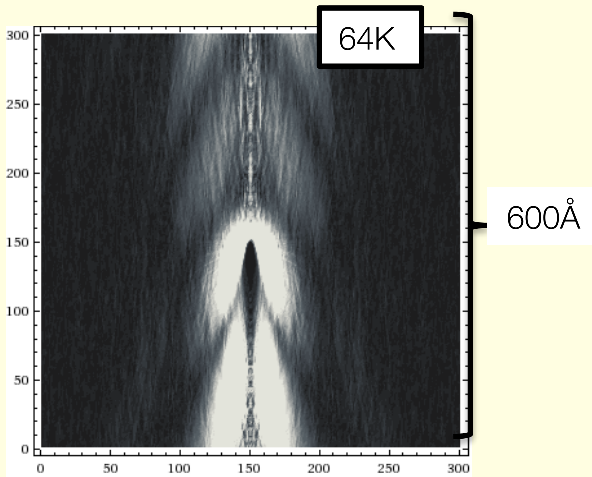
n=1.03X10^{20}/cc, T=1.088 eV, N=64K, L= 853 Å, Z=-20
v=50Å/fs = 11.4 v/v_{th} along x

interaction with the wakefield
from periodic replicas is obvious

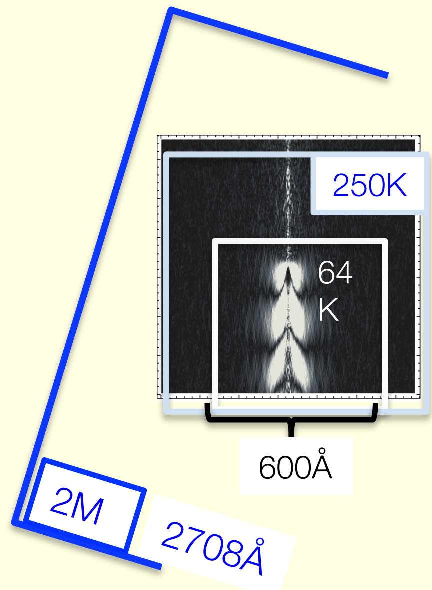
rotate the projectile trajectory to stagger
the periodic array of wakefields



density, n(r)



current density, |j(r)|



verify that dE/dx agrees
between sizes of 64K and 2M

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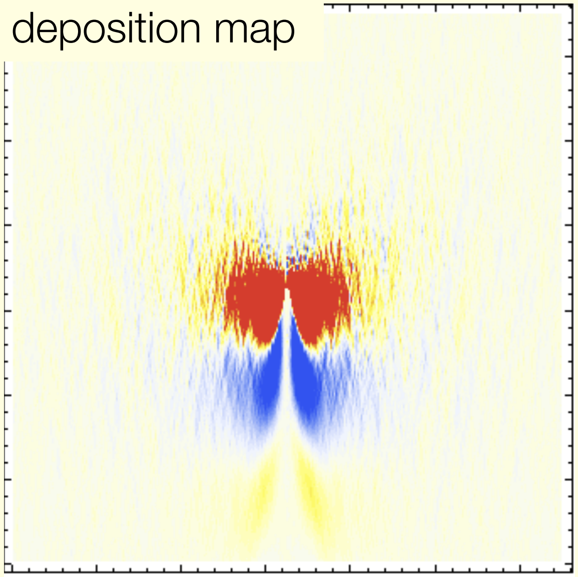
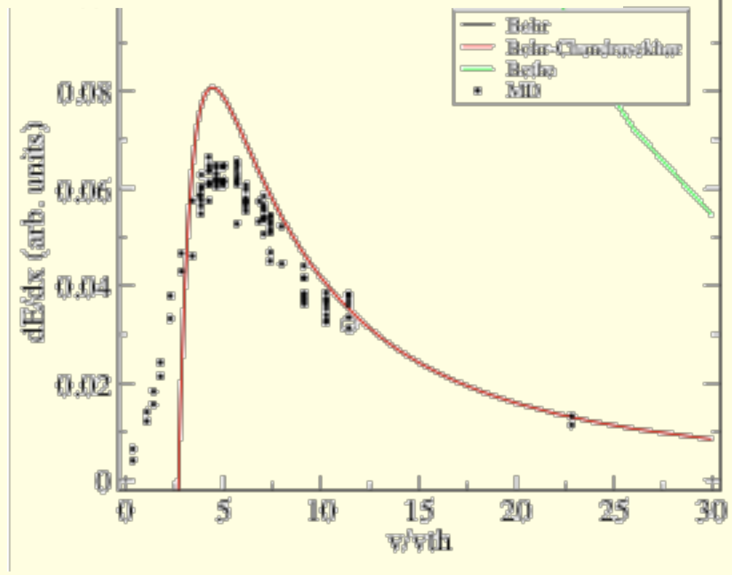
MD is then mined to obtain useful information

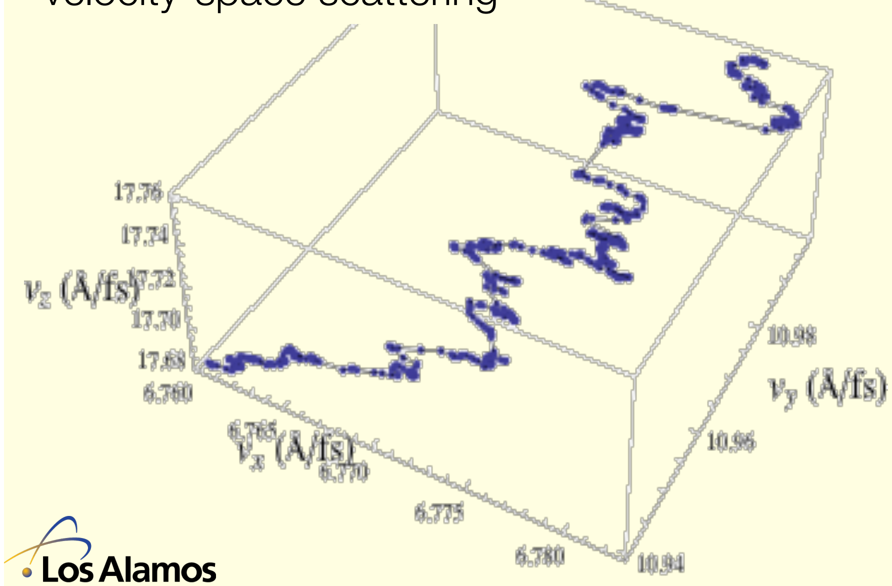
energy deposition map



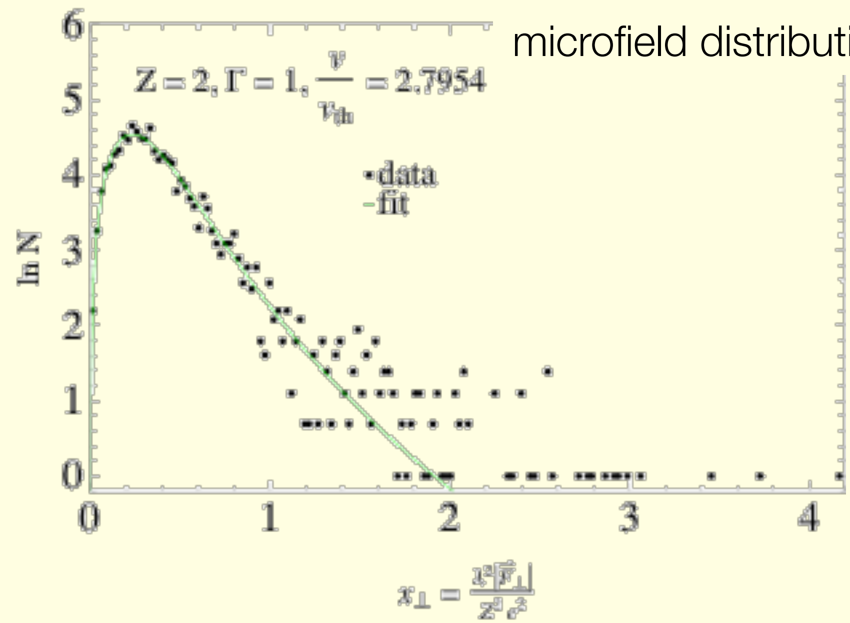
dE/dx vs. v for Z=-10 in e⁻ gas, Γ =1



velocity-space scattering



microfield distribution



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We chose a range of models

- Born (LB) models (static, dynamic, and variants)
- T-matrix (numerical cross section in Yukawa potential)
- Two new T-matrix formulations (better screening)
    - Poisson-Boltzmann
    - Hypernetted Chain
- Velocity-dependent T-matrix, and its embellishments
- Formal connection to diffusive transport

Static and Dynamic Born Models

Dynamic Born (Lenard-Balsecu):

$$\frac{\partial \langle E \rangle}{\partial t} = \frac{2Ze^2}{\pi v} \int_0^{k_M} \frac{dk}{k} \int_{-kv}^{kv} d\omega \omega Im \epsilon^{-1}(k,\omega)$$

$$\epsilon = 1 + \frac{1}{\lambda^2 k^2} \left(1 - u\sqrt{\frac{\pi}{2}} e^{-u^2/2} \left(\text{erfi} \left(\frac{u}{\sqrt{2}} \right) + i \right) \right)$$

$$u = \frac{\omega}{k v_{th}} \qquad k_M = \frac{2\pi T}{Ze^2} \left(1 + \frac{v^2}{v_{th}^2} \right)$$

Static Born (perturbative screened Coulomb):

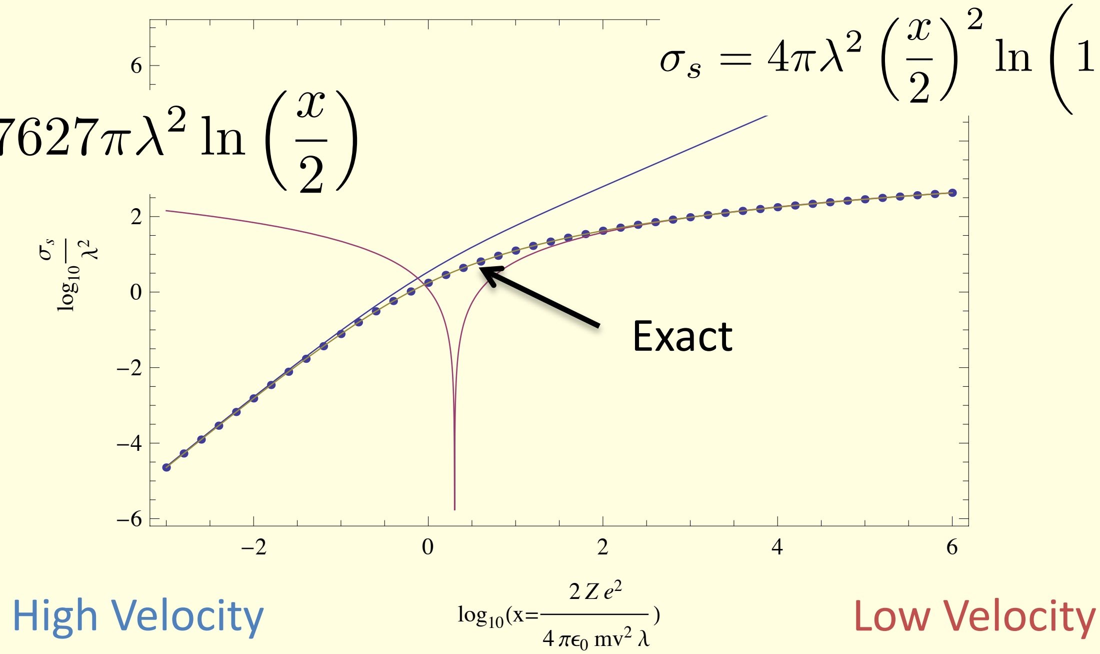
$$\epsilon^{-1}(k,\omega) \to \frac{\epsilon^*(k,\omega)}{|\epsilon(k,0)|^2}$$

T-matrix models: Infinite-Order in Scattering

$$\sigma_s = 4\pi\lambda^2 \left(\frac{x}{2}\right)^2 \ln\left(1 + \frac{2}{x}\right)$$

$$\sigma_s = 0.787627\pi\lambda^2 \ln\left(\frac{x}{2}\right)$$

$$v_{pt}(r) = \frac{Ze^2}{r} e^{-r/\lambda}$$



Gould-Dewitt class:

$$\frac{\partial\langle E\rangle}{\partial t} = \frac{\partial\langle E\rangle}{\partial t}^{\text{static}}_{\text{T-Matrix}} + \frac{\partial\langle E\rangle}{\partial t}^{\text{dynamics}}_{\text{Born}} - \frac{\partial\langle E\rangle}{\partial t}^{\text{static}}_{\text{Born}}$$

Note: Models in this class are completely convergent. No cutoffs, no Coulomb logarithm.

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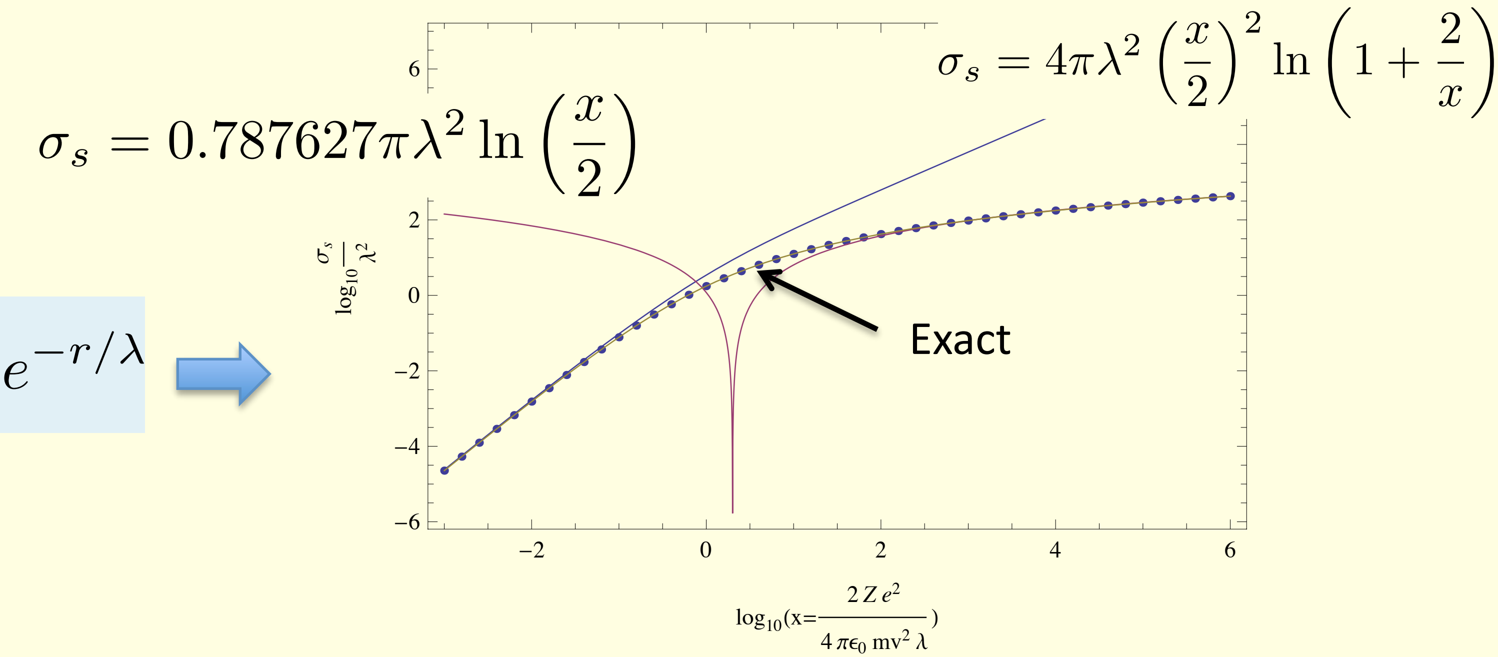
Extended T-matrix models: Effects of Velocity to All Orders

$$v_{pt}(r) = \frac{Ze^2}{r} e^{-r/\lambda}$$



$$\lambda_Z = \lambda\sqrt{1 + \frac{v^2}{v_{th}^2}}$$

"Zwicknagel"

In words:

1. Compute screening length in plasma.
2. For each velocity, form modified screening length.
3. Numerically compute cross section.
4. Compute stopping power.

Diffusion and the Low-Velocity Limit

The diffusion coefficient can be written exactly in statistical mechanics as:

$$D = \frac{1}{3}\int_0^\infty \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle$$

In particular, MD is really good at calculating this for moderate to strong coupling.

Various fits exist in the literature.

$$\frac{D}{\omega_E a^2} = \alpha \left(\frac{\Gamma}{\Gamma_m} - 1 \right)^\beta + \gamma$$

Now, back to stopping power: in the low-velocity limit when the projectile-target mass ratio is large, we have exactly:

$$\frac{dE}{dx} = \left(\frac{T}{D} \right) v$$

PHYSICS OF PLASMAS VOLUME 7, NUMBER 11 NOVEMBER 2000

Molecular dynamics evaluation of self-diffusion in Yukawa systems

H. Ohta and S. Hamaguchi
Department of Fundamental Energy Science, Kyoto University, Gokasho, Uji, Kyoto 611-0011, Japan

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Nuclear Instruments and Methods in Physics Research B 96 (1995) 626–632
NIM B Beam Interactions with Materials & Atoms

Electronic stopping of ions in the low velocity limit

James W. Dufty *, Mikhail Berkovsky
Department of Physics, University of Florida, Gainesville, FL 32611, USA

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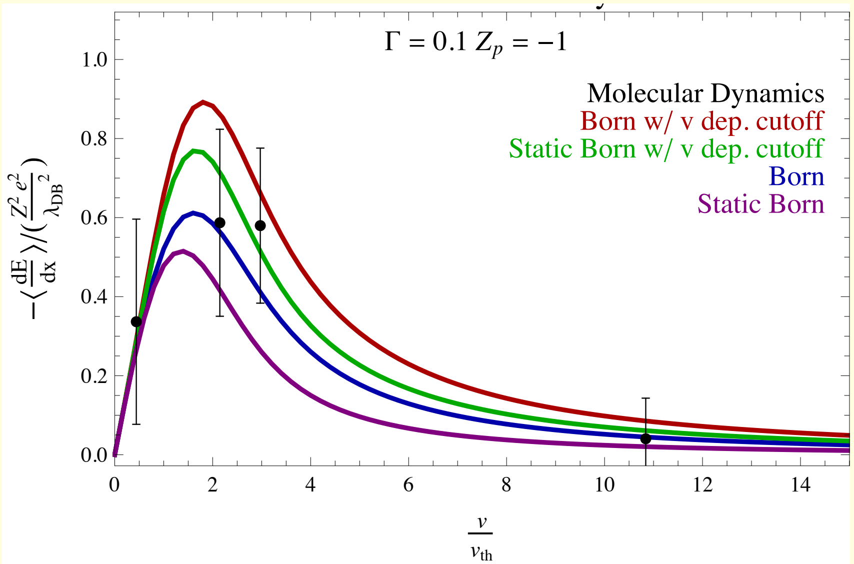
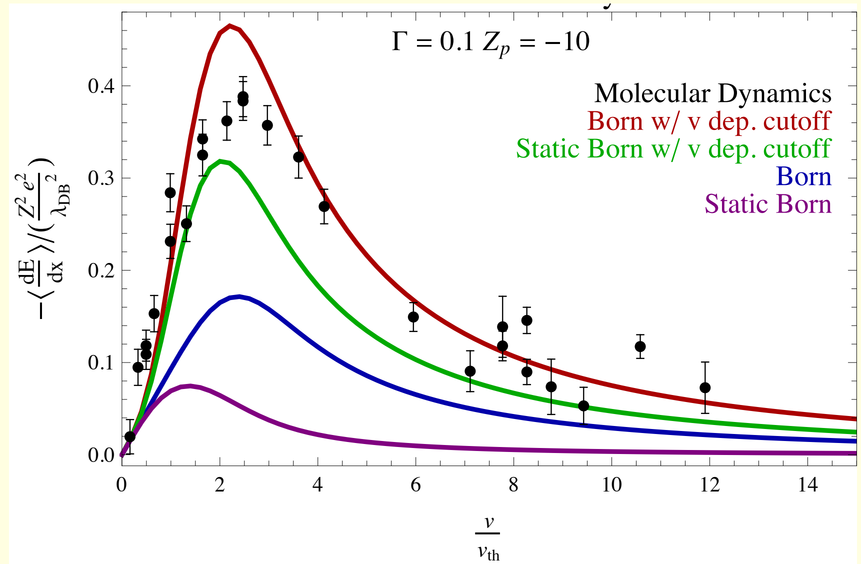
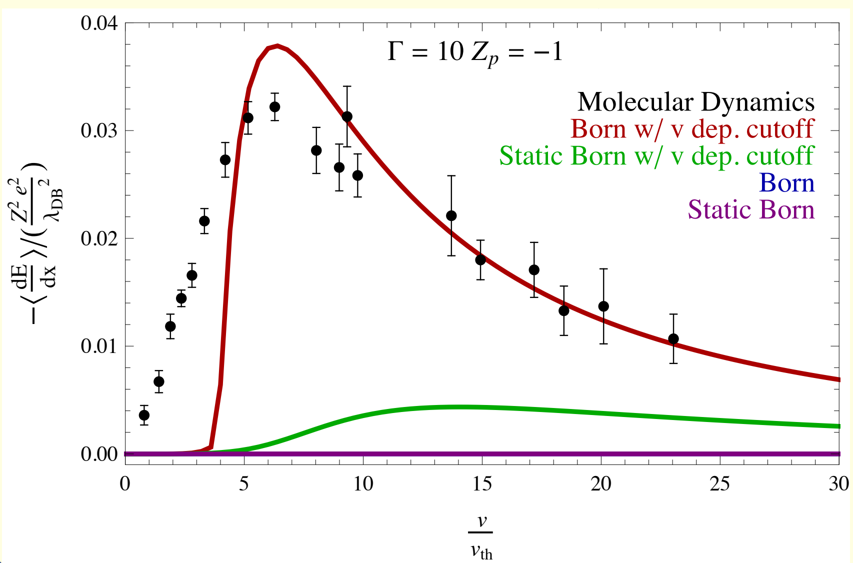
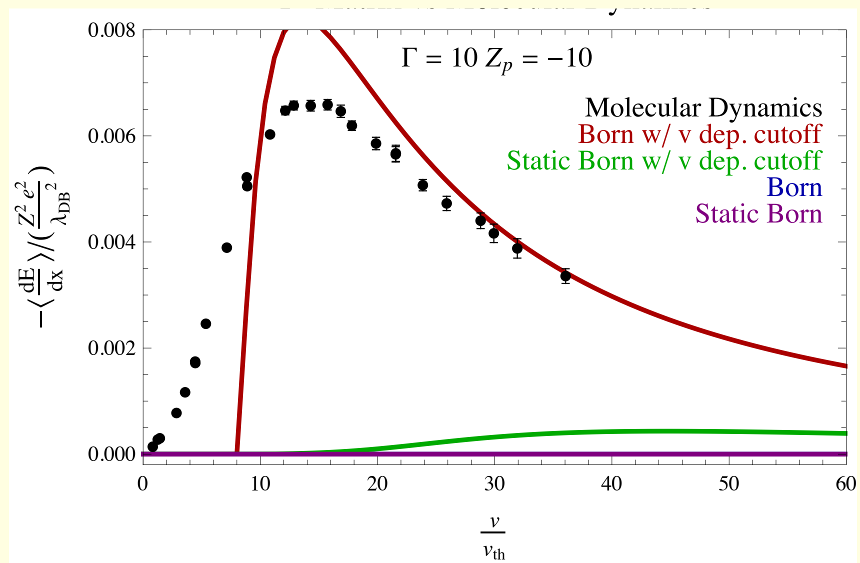
Born and MD Results









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Static and Dynamic Born Models: Conclusion

Dynamic Born (Lenard-Balsecu):

$$\frac{\partial\langle E\rangle}{\partial t} = \frac{2Ze^2}{\pi v}\int_0^{k_M}\frac{dk}{k}\int_{-kv}^{kv} d\omega\omega Im\epsilon^{-1}(k,\omega)$$

$$\epsilon = 1 + \frac{1}{\lambda^2 k^2}\left(1 - u\sqrt{\frac{\pi}{2}}e^{-u^2/2}\left(\mathrm{erfi}\left(\frac{u}{\sqrt{2}}\right) + i\right)\right)$$

$$u = \frac{\omega}{kv_{th}} \qquad k_M = \frac{2\pi T}{Ze^2}\left(1 + \frac{v^2}{v_{th}^2}\right)$$

Yes!

Static Born (perturbative screened Coulomb):

$$\epsilon^{-1}(k,\omega) \to \frac{\epsilon^*(k,\omega)}{|\epsilon(k,0)|^2}$$

No!

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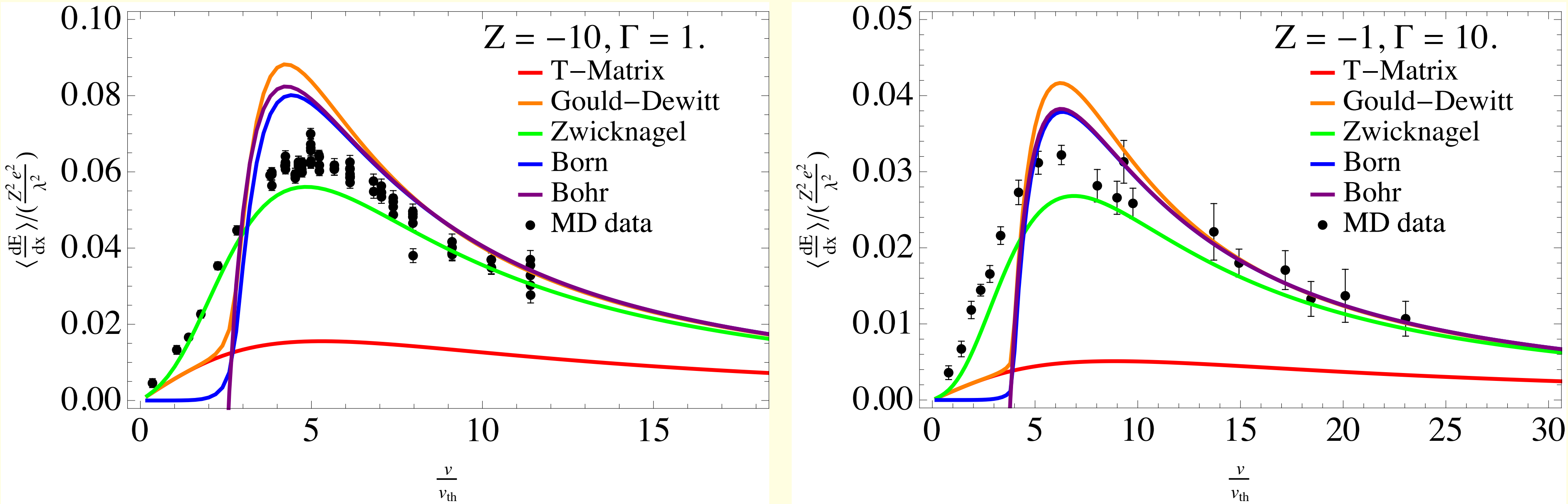
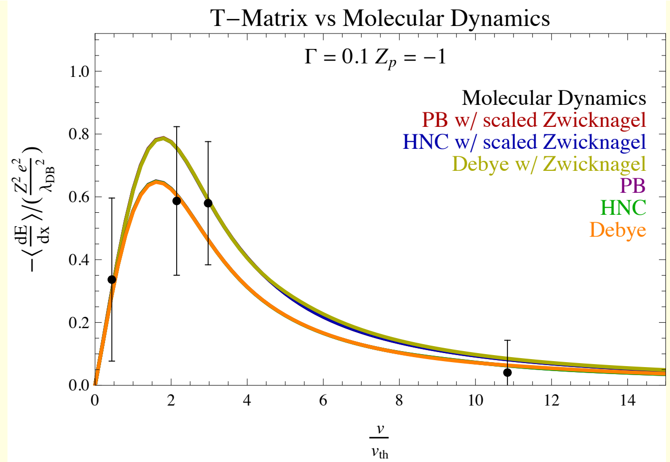
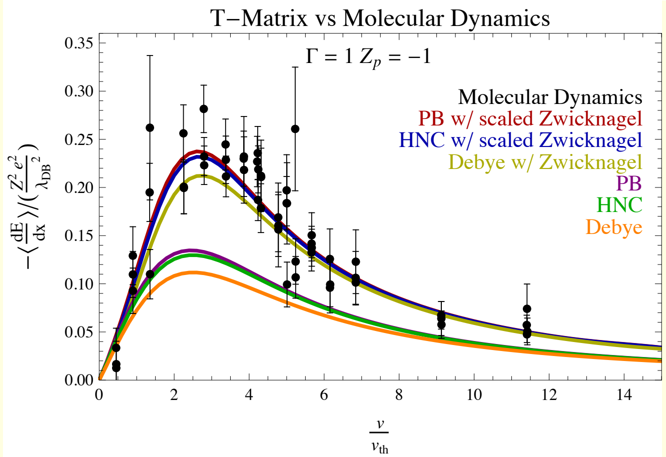
Gould DeWitt Results

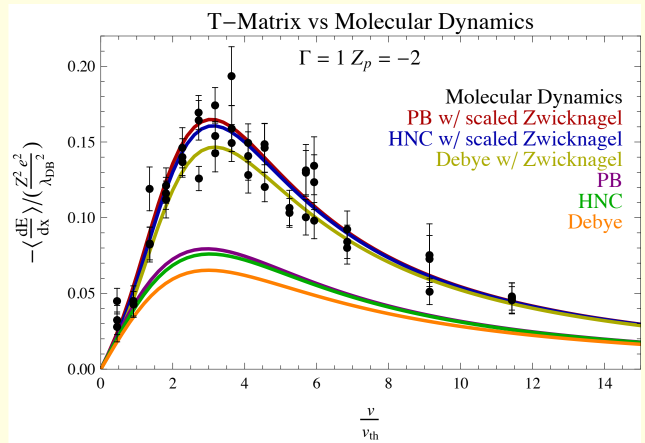


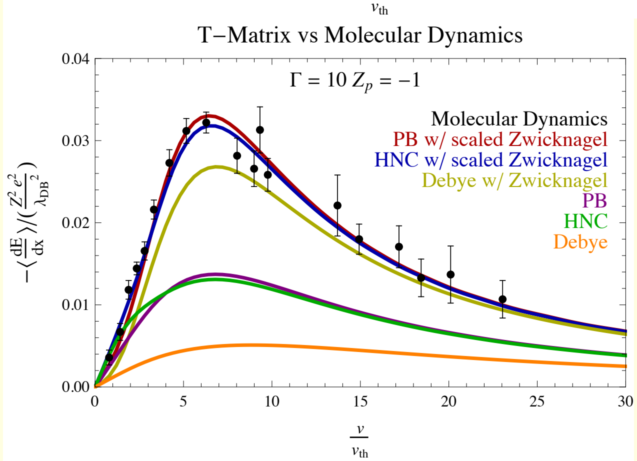
- This model does no harm.
- When it makes a difference is also when it fails.

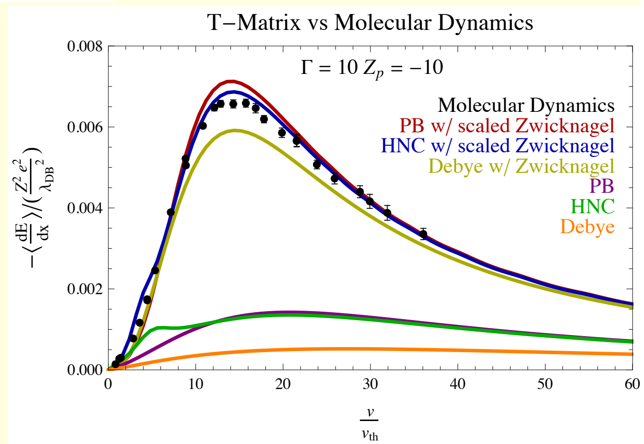
T-matrix Results



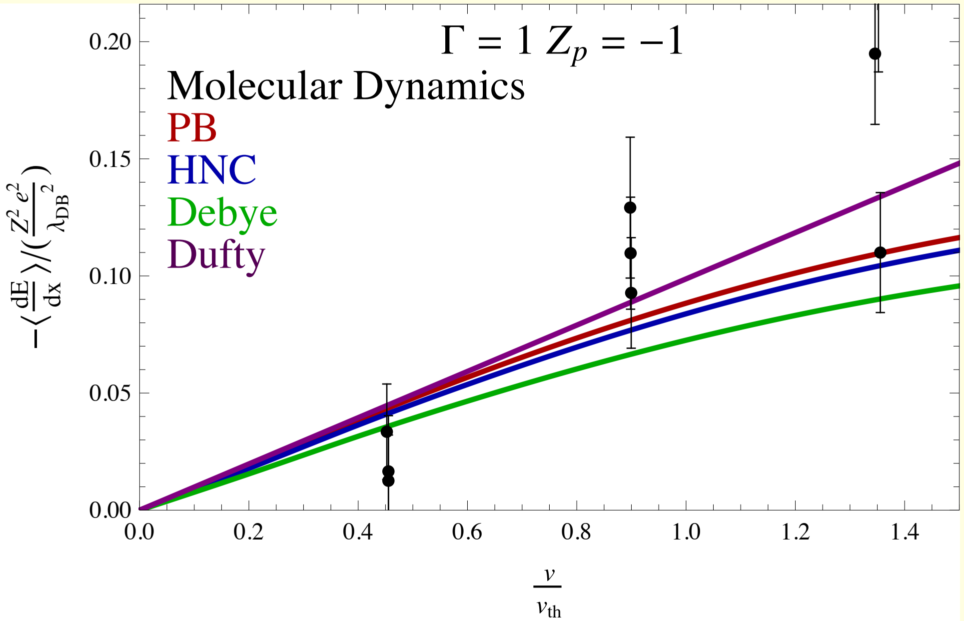






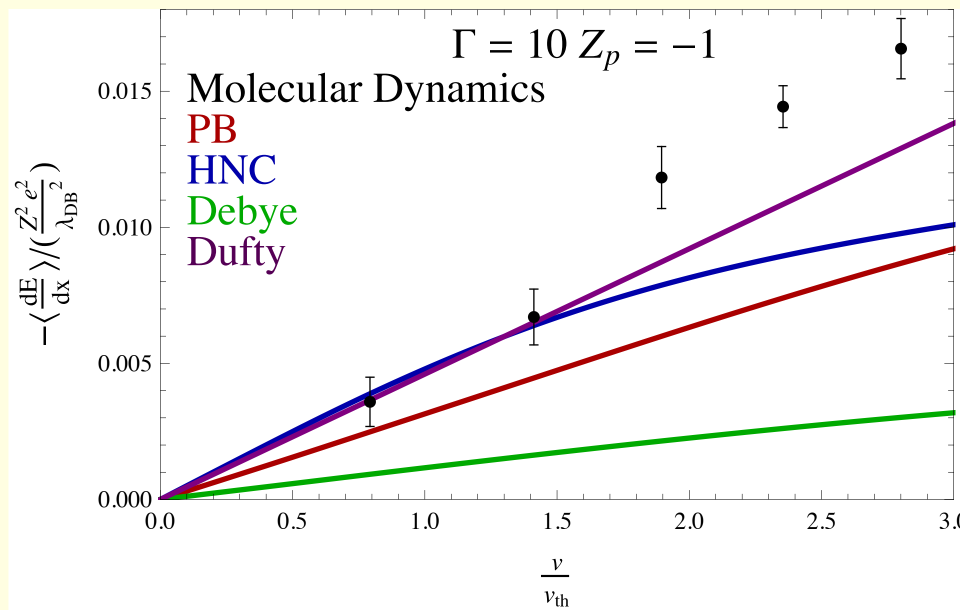


Low-Velocity and Diffusion



Diffusion model works very well where it should.

But, we now know where it breaks down.



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Summary and Outlook

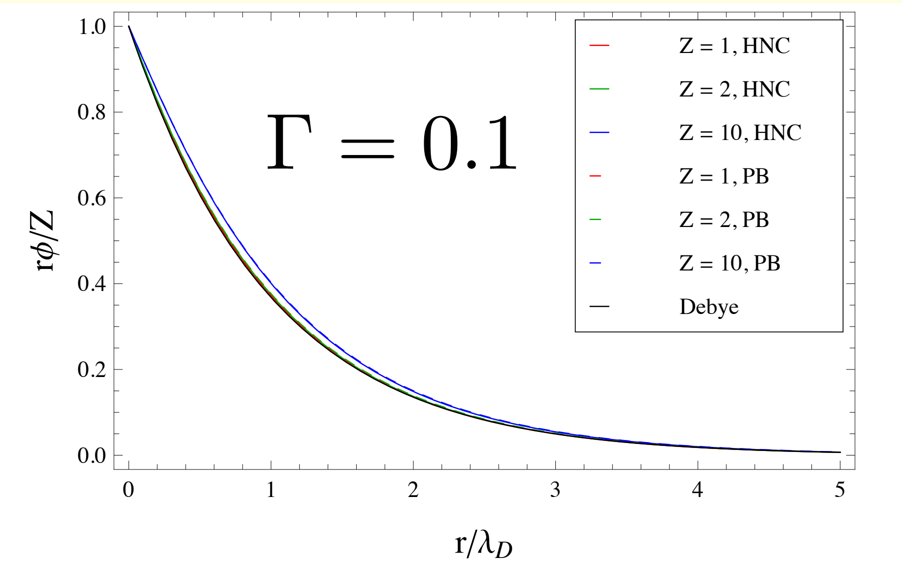
- We have performed a set of accurate MD simulations of charged-particle stopping that spans the range from weak to moderate to strong coupling in both target coupling and target-projectile coupling.

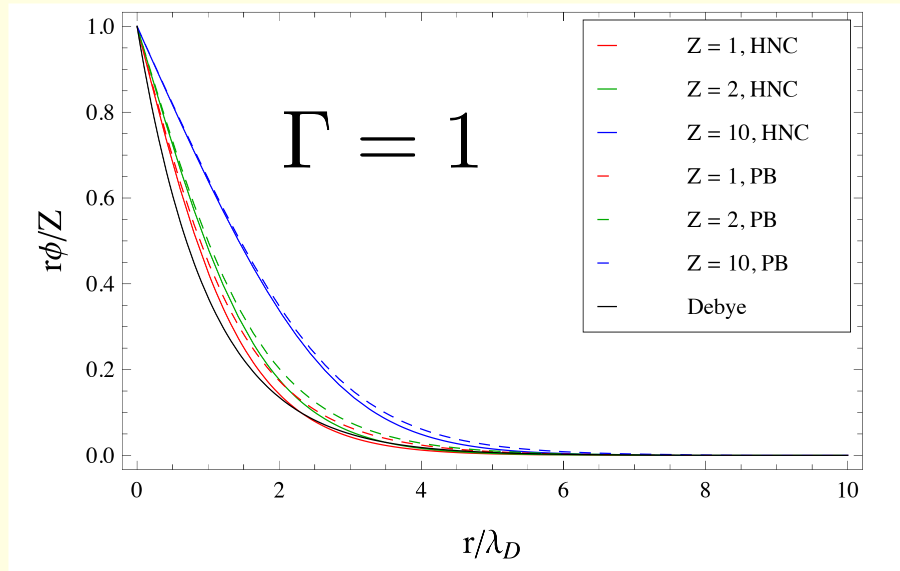
- More is on the way! We are still not happy with error bars on all parts of the data set.

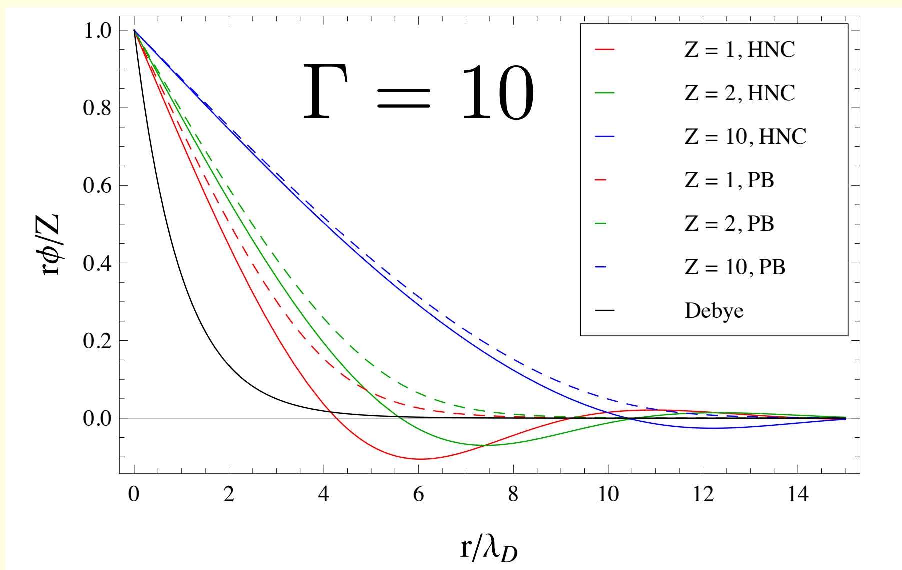
- Once published, we hope our data will provide years of stringent tests for the stopping power community and, more broadly, the plasma kinetic theory community.

- We have compared with a wide range of theoretical models. While we find roughly what we expect, we now have very precise rules about what we know and don't know.

Nonlinear (Numerical) Screening Potentials







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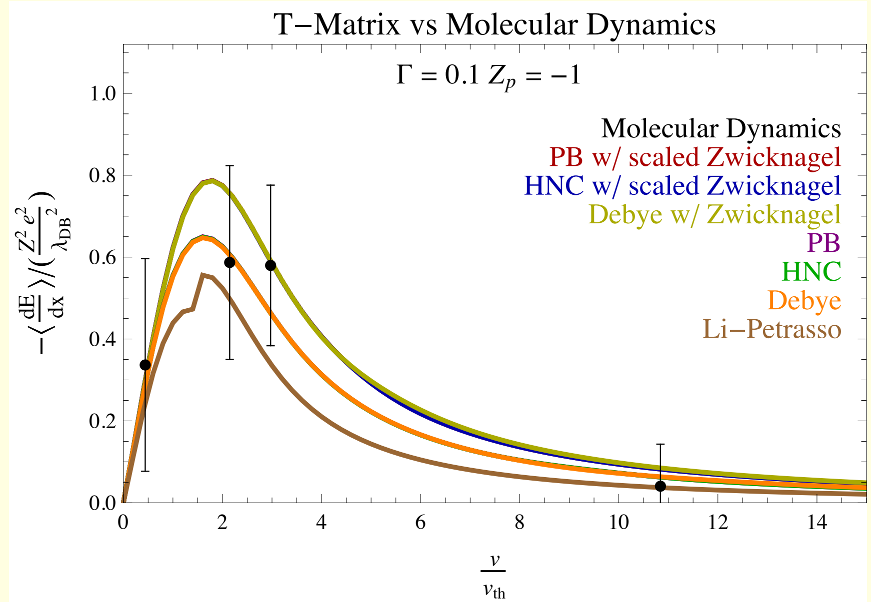
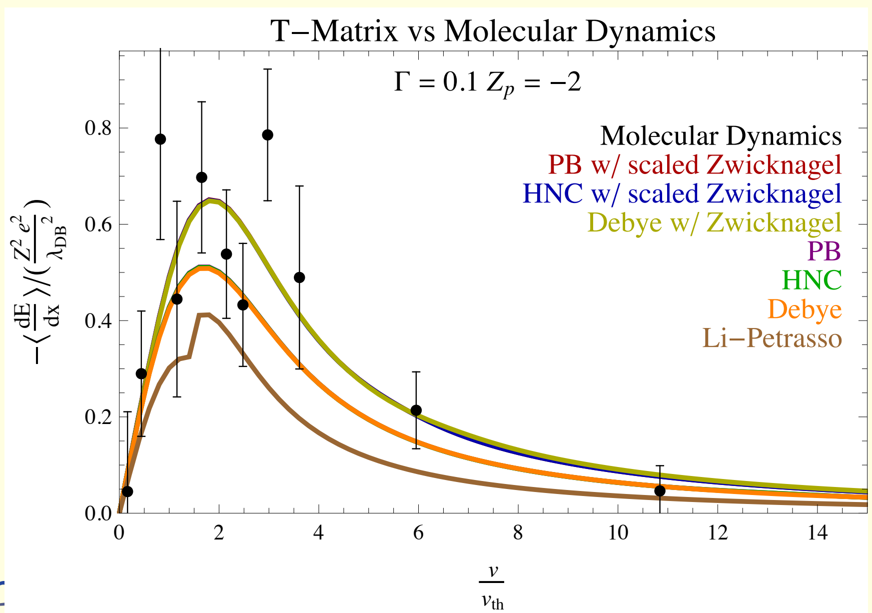
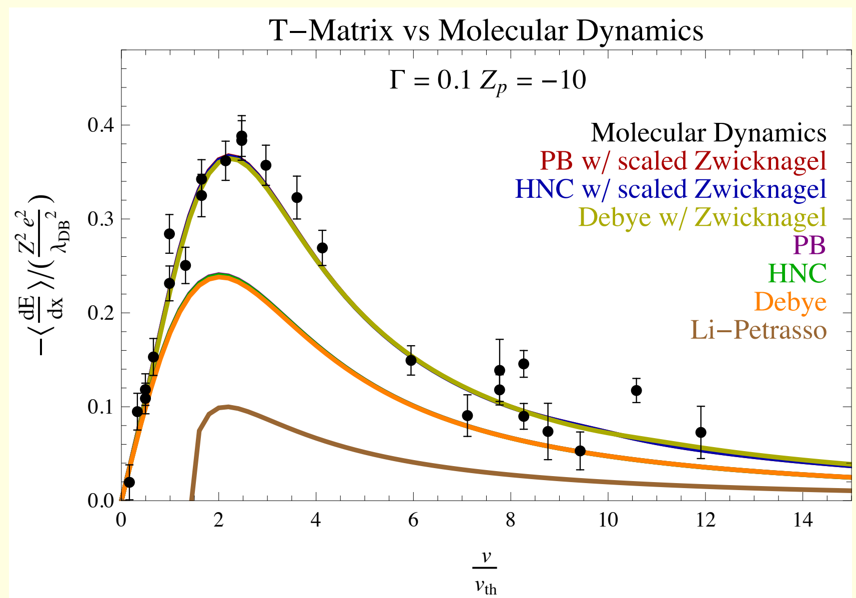
Li-Petrasso Model

A model intended for:

- Weakly coupled plasma
- Moderate scattering







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Today, there is a renewed interest in transport phenomena.

1. When does any formulation of hydrodynamics break down?
   1. When do we need multi-species hydro?
   2. At what length scales do spatial gradients matter?
   3. At what time scales do temporal gradients matter?
   4. Are current highly-resolved calculations approaching their limits?
2. What forms do the “gradient corrections” take?
   1. From Euler to Navier-Stokes to what?
   2. What are the transport coefficients and what are their values?
3. Are there “kinetic effects” (physics not handled by gradient corrections)?
   1. Non-thermal distributions.
   2. Finite-mean-free paths.

Our Approach: Go Back to Basics

In practice, we always use kinetic models.

$$\frac{\partial}{\partial t} f(\mathbf{r}, \mathbf{v}, t) + \mathbf{v} \cdot \nabla f(\mathbf{r}, \mathbf{v}, t) + m^{-1} \mathbf{F}_{mf} \cdot \nabla_v f(\mathbf{r}, \mathbf{v}, t) = \mathcal{C}[f(\mathbf{r}, \mathbf{v}, t)]$$

Several issues arise:

- Often we do not want to solve a kinetic equation.
- Even we we do, there are numerical issues.
- All of the physics uncertainty enters through the collision term.
- Without a complete understanding of the collisions, hydro models may suffer.

What are typical plasma collision treatments?

- Nothing (Vlasov).
- Fokker-Planck.
- Linear models (Lenard-Bernstein, linear Boltzmann, etc.).
- Non-linear models (BGK).
- Lenard-Balescu.
- Etc.

There are three reasons that we care about stopping power.

1. Stopping power is ubiquitous problem in physics that many, many other scientific communities have paid a lot of attention to.

2. Fast charged particles are created in fusion plasmas and are needed to heat the fuel, or be used as a diagnostic of the fuel.

3. The stopping power is a *velocity-resolved* transport issue. Stopping power is detailed in this sense: we do not average over a distribution to get an integrated quantity; it is always a "mean-free-path" effect.

Transport and Thermonuclear Burn

radiation, temperature relaxation, electron thermal conduction, stopping power, diffusive mixing, tail depletion, etc.

$$\frac{\partial T_i}{\partial t} = \frac{1}{C_{vi}}\left[\dot{S}_i - \left(P_i + q + \frac{\partial I_i}{\partial v}\right)\frac{\partial v}{\partial t} - A_{ie}(T_i - T_e) + \frac{v}{r^2}\frac{\partial}{\partial r}\left(r^2 K_i \frac{\partial T_i}{\partial r}\right)\right],$$

$$\frac{\partial T_e}{\partial t} = \frac{1}{C_{ve}}\left[\dot{S}_e - \left(P_e + \frac{\partial I_e}{\partial v}\right)\frac{\partial v}{\partial t} - A_{er}(T_e - T_r) + A_{ie}(T_i - T_e) + \frac{v}{r^2}\frac{\partial}{\partial r}\left(r^2 K_e \frac{\partial T_e}{\partial r}\right)\right],$$

$$\frac{\partial T_r}{\partial t} = \frac{1}{C_{vr}}\left[-\left(P_r + \frac{\partial I_r}{\partial v}\right)\frac{\partial v}{\partial t} + A_{er}(T_e - T_r) + \frac{v}{r^2}\frac{\partial}{\partial r}\left(r^2 K_r \frac{\partial T_r}{\partial r}\right)\right].$$

EOS

radiation

T-relaxation

thermal conduction

stopping power